Dr. H. E. H. Bright

CANADA

DEPARTMENT OF MINES AND TECHNICAL SURVEYS

MINES BRANCH

OTTAWA

MINERAL SCIENCES DIVISION

INTERNAL REPORT MS-65-97

ATTENDANCE AT THE JOINT MEETING OF THE AMERICAN CRYSTALLOGRAPHIC ASSOCIATION AND THE MINERALOGICAL SOCIETY OF AMERICA, GATLINBURG, TENNESSEE, JUNE 27 - JULY 2, 1965

by

J. F. Rowland
Physical Chemistry Section

23 September 1965

MINES BRANCH

Mineral Sciences Division

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(Author) John F. Rowland

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Mineral Sciences Division Internal Report MS-65-97

ATTENDANCE AT THE JOINT MEETING OF THE AMERICAN CRYSTALLOGRAPHIC ASSOCIATION AND THE MINERALOGICAL SOCIETY OF AMERICA, GATLINBURG, TENNESSEE, JUNE 27 -JULY 2, 1965

by

J. F. Rowland *

INTRODUCTION

This report covers the attendance of Mr. J. F. Rowland at the joint meeting of the American Crystallographic Association and the Mineralogical Society of America, which was held in Gatlinburg, Tennessee from Sunday, June 27 to Friday, July 2, 1965.

Attendance at the meeting required the writer to be absent from his office in Ottawa for four working days, and to attend technical sessions on a statutory holiday (July 1). Travel between Ottawa and Knoxville, Tennessee was by air (Air Canada and United Air Lines) via Toronto and Cleveland. The flight tickets were obtained using the Mines Branch credit card, and the cost of the return trip was $150.00. Approximately $115.00 was spent by the writer in addition to the plane fare, and this sum includes the cost of registration, accommodation, meals, local transportation, and certain functions associated with the

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* Senior Scientific Officer, Physical Chemistry Section, Mineral Sciences Division, Mines Branch, Department of Mines and Technical Surveys, Ottawa, Canada.

meeting. The writer's wife accompanied him to Gatlinburg at his own expense.

The meeting included eighteen sessions of technical papers, thirteen sponsored by the American Crystallographic Association, three by the Mineralogical Society of America, and two jointly by both organizations. A total of 170 papers, including four invited by the A.C.A., were presented, and represented the work of about 250 authors and co-authors. All the sessions were held in the Civic Auditorium, Gatlinburg, in one of three assembly halls. Since generally two, and on occasion three, sessions were held simultaneously, it was impossible for one to be present for all the papers. Also, since a strict timetable was not adhered to, it was difficult to apportion attendance between simultaneous sessions in order to hear certain papers that were supposed not to conflict. The writer attended 74 papers, including the four invited ones, all of interest to him to some degree, but he was unable to be present at several others that were of interest to him and his co-workers at the Mines Branch, due to conflict in scheduling.

In addition to the technical sessions, various meetings were held, including the following: U.S.A. National Committee for Crystallography, A.S.T.M. Committee on Chemical Analysis by X-ray Diffraction, and A.C.A. Business Meeting. On June 30 and July 1, four all-day field trips were arranged by the M.S.A. Daily trips to the Oak Ridge National Laboratory were also available for those registered at the meeting. The writer did not participate in these meetings or field trips.

An exhibition of equipment used for X-ray and electron diffraction was sponsored by the meeting, and representatives of many manufacturers were present with displays of their latest equipment. Of particular interest to the writer were the automated Supper single-crystal diffractometer and the Matthews X-ray Coordinate Index of the American Society for Testing and Materials.

TECHNICAL PAPERS ATTENDED BY THE WRITER

The following tabulation includes only those papers that the writer attended, and is not meant to be a complete record of the Gatlinburg meeting. The titles and abstracts of all the papers are available from several employees of Mineral Sciences Division, including the writer. In the case of papers with more than one author, the name of the one presenting the paper is underlined.

Monday Morning, June 28

WELCOME: Dr. Alvin M. Weinberg, Director, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

OPENING OF MEETING: Dr. Henri A. Levy, President of A.C.A., Oak Ridge National Laboratory, Oak Ridge, Tennessee.

A.C.A. SESSION A: INTERFERENCE, DIFFRACTION, SCATTERING (B. W. Batterman presiding): INVITED PAPERS:

A-1: "An X-ray Interferometer", U. Bonse and M. Hart, Materials Science Center, Cornell University, Ithaca, New York.

A-2: "Peaks and Centroids in Accurate Lattice-Parameter Determination", A. J. C. Wilson, University College, Cardiff, Wales, and Georgia Institute of Technology, Atlanta, Georgia.

A-3: "Diffuse Scattering by Neutron Irradiated Quartz", A. Guinier, Université de Paris, France.

A.C.A. SESSION A: CONTRIBUTED PAPERS:

A-4: "A Spark Chamber Single Crystal X-ray Diffractometer". J. P. Cowan, W. M. Macintyre, R. Thomas, Chemistry Department, University of Colorado, Boulder, Colorado.

A-5: "Intrinsic and Systematic Multiple Diffraction", R. D. Burbank, Bell Telephone Laboratories Incorporated, Murray Hill, New Jersey.

A-6: "A New X-ray Monochromator Configuration for Single Crystal Diffractometry", T. C. Furnas, Jr. and D. W. Beard, Picker X-ray Corporation, Cleveland, Ohio.

A-7: "Anomalous Transmission of Continuous X-ray Spectrum through Silicon", R. E. DeWames, G. W. Leham, W. G. Brammer, D. O. Thompson and P. C. Romo, North American Aviation Science Center, Thousand Oaks, California.

A-8: "Variance of Absorption Effects Observed in Integrated Intensity Measurements of Sodium Chloride and Silicon Single Crystals", G. J. Klems, Republic Steel Corporation, Research Center, Independence, Ohio; and C. J. Polk, Department of Metallurgical Engineering, Illinois Institute of Technology, Chicago, Illinois.

Monday Evening, June 28

A.C.A.-M.S.A. JOINT SESSION JA: PHYSICAL METHODS, MORPHOLOGY (D. McLachlan presiding):

JA-1: "High Dispersion and High Intensity Powder Diffractometry", W. Parrish, Philips Laboratories, Briarcliff Manor, New York.

JA-2: "X-ray Diffraction at Ultra-High Pressure and Temperature", W. G. Field, Air Force Cambridge Research Laboratory, L. G. Hanscom Field, Bedford, Massachusetts.

JA-3: "The Crystal Substructure in BeO", D. K. Smith and H. W. Newkirk, Lawrence Radiation Laboratory, University of California, Livermore, California.

JA-4: "Observations on the Morphology and Growth of Colloidal Crystals of Hydrated Tungsten Oxide by Electron Microscopy of their Ultrathin Sections", J. H. L. Watson, Edsel B. Ford Institute for Medical Research, Detroit, Michigan.

JA-5: "Determination of Proton Positions in Crystals by Infrared Spectroscopy", W. B. White, Materials Research Laboratory, Pennsylvania State University, University Park, Pennsylvania.

JA-6: "Fourier Technique for the Analysis of Zeeman NQR Zero Crossing Data", G. E. Peterson, Bell Telephone Laboratories Incorporated, Murray Hill, New Jersey.

JA-7: "Evaluation of Thermal Parameters for Silicon, Aluminum, and Oxygen Atoms in Silicates", C. W. Burnham, Geophysical Laboratory, Carnegie Institution of Washington, Washington, D. C.

Tuesday Morning, June 29

A.C.A. SESSION C: PROPERTIES OF CRYSTALS, THEORY AND EXPERIMENT

(W. Parrish presiding):

C-1: "Theoretical Coefficients of Expansion of Crystals" D. McLachlan, Jr., Department of Mineralogy, Ohio State University, Columbus, Ohio.

C-2: "Nonbonded Interatomic Potential Functions from Packing Analyses of Molecular Crystals", D. E. Williams, Iowa State University, Ames, Iowa.

C-6: "The Positions of the Hydrogen Atoms and their Role in the Ferroelectric Behavior of Colemanite", F. N. Hainsworth and H. E. Petch, Departments of Physics and Metallurgy, Hamilton College, McMaster University, Hamilton, Ontario.

C-7: "LEED Study of (110) Cleavage Faces of II-VI Compounds, I. CdTe", L. Feinstein, M. Taylor, J. Keil, D. P. Shoemaker, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts.

M.S.A. SESSION III: MINERAL OCCURRENCES, PARAGENESIS, CRYSTAL-CHEMICAL RELATIONS (R. Dietrich and E. Roedder co-chairmen) :

III-3: "Phase Relations in the Silver-Tellurium System", F. C. Kracek, C. J. Ksanda and L. J. Cabri, Mineral Sciences Division, Department of Mines and Technical Surveys, Ottawa, Ontario.

III-4: "Clinohumite from Cotopaxi, Colorado", V. J. Hurst and C. A. Salotti, Department of Geology, University of Georgia, Athens, Georgia.

III-8: "An Unusual Dolomitic Basal Facies of the Chattanooga Shale in the Flynn Creek Structure, Tennessee", D. J. Roddy, Division of Geological Sciences, California Institute of Technology, Pasadena, California, and U. S. Geological Survey, Flagstaff, Arizona.

III-10: "Composition and Distribution of Feldspars in the Muskox Instrusion, N. W. T., Canada", G. Pouliot, Geological Survey of Canada, Department of Mines and Technical Surveys, Ottawa, Ontario.

Tuesday Afternoon, June 29

A.C.A. SESSION E: BIOLOGICAL AND ORGANIC STRUCTURES (D. Harker presiding) :

E-1: "Recent Results of the X-ray Investigation of Muscle Lactic Dehydrogenases", B. A. Jeffery, P. Main and M. G. Rossmann, Department of Biological Sciences, Purdue University, Lafayette, Indiana.

E-2: "A One Dimensional Example of the Molecular Replacement Method", P. Main and M. G. Rossmann, Department of Biological Sciences, Purdue University, Lafayette, Indiana.

E-3: "Use of a Flow Cell in Enzyme Single Crystal Studies" H. W. Wyckoff, F. M. Richards and D. Tsernoglou, Yale University, New Haven, Connecticut.

E-4: "Diffraction Studies of Ribonuclease-S and Inhibitor-Enzyme Complexes", F. M. Richards, H. W. Wyckoff, M. Doscher, D. Tsernoglou and T. Inagami, Yale University, New Haven, Connecticut.

A.C.A. SESSION F: INORGANIC STRUCTURES (J. S. Kasper presiding):

F-4: "The Structure of Sodium Triphosphate Hexahydrate, $Na_5P_3O_{10}.6H_2O$", D. R. Dyroff and E. W. Hughes, California Institute of Technology, Pasadena, California.

F-5: "A Neutron Diffraction Investigation of Hypophosphorous Acid", J. Williams and S. W. Peterson, Department of Chemistry, Washington State University, Pullman, Washington.

F-6: "The Crystal Structure of Eu_3O_4", R. C. Rau, General Electric Company, Nuclear Materials and Propulsion Operation, Cincinnati, Ohio.

F-7: "Data for $LaTaO_4$, A new Structure Type, and a Series of New Compounds with the $PbNb_2O_6$ Structure, of the Composition $K_{O.5}M_{O.5}Ta_2O_6$, where M is a Rare Earth", G. M. Wolten and A. B. Chase, Aerospace Corporation, Los Angeles, California.

F-8: "Thorium Phosphide Type Rare Earth Compounds", F. Holtzberg, Y. Okaya and N. Stemple, I.B.M. Research, Yorktown Heights, New York.

F-9: "Neutron Diffraction Study of Single Crystal Calcia Stabilized Zirconia", W. L. Roth, General Electric Research Laboratory, Schenectady, New York.

F-10: "The Magnetic Structures of Fe_2SiO_4 and Mn_2SiO_4", D. E. Cox and B. C. Frazer, Brookhaven National Laboratory, Upton, New York; I. Almodovar and M. I. Kay, Puerto Rico Nuclear Center, Mayaguez, Puerto Rico.

Wednesday Morning, June 30

A.C.A. SESSION G: ORGANIC STRUCTURES (A. L. Patterson presiding):

G-4: "The Crystal Structure of Tetraphenylarsonium 1, 1, 5, 5, 5-pentacyano-4-fluoro-2-azapentadienide: An Example of Chemical Analysis by X-ray Diffraction", G. J. Palenik, U. S. Naval Ordnance Test Station, China Lake, California.

G-8: "The Crystal and Molecular Structure of a Previously Unidentified Diels-Alder Adduct", R. E. Davis, Roswell Park Memorial Institute, Buffalo, New York; and A. Tulinsky, Sterling Chemistry Laboratory, Yale University, New Haven, Connecticut.

G-9: "The Structure of a Diels-Alder Adduct of an Azepine", J. H. van den Hende and A.S. Kende, Lederle Laboratories, A Division of American Cyanamid Company, Pearl River, New York.

G-10: "The Crystal Structure of 2,2-diphenyl-4,4,6,6-tetrachlorocyclo-triphosphazatriene", N. V. Mani, F. R. Ahmed and W. H. Barnes, Pure Physics Division, National Research Council, Ottawa, Ontario.

A.C.A. SESSION H: INORGANIC STRUCTURES (S. W. Peterson presiding):

H-1: "Crystal Structure of Ferroelectric Lithium Metaniobate, $LiNbO_3$", S. C. Abrahams, J. M. Reddy and J. L. Bernstein, Bell Telephone Laboratories Incorporated, Murray Hill, New Jersey.

H-2: "Non-Centrosymmetric Structures in the Hexagonal Ferrite Group", J. A. Kohn and D. W. Eckart, U. S. Army Electronics Laboratories, Fort Monmouth, New Jersey.

H-4: "Refinement of the Structure of Li_2BeF_4", J. H. Burns and E. K. Gordon, Reactor Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

H-5: "On the Shape of the Tl^+ ion in Thallium Halides and Thallium Halide Alkali Halide Solid Solutions", S. Hafner, Institute for the Study of Metals, University of Chicago, Chicago, Illinois.

H-6: "The Crystal Structure of Monoclinic Sulfur", D. E. Sands, University of Kentucky, Lexington, Kentucky.

H-11: "High Pressure Single Crystal Studies of Ice VI and Ice VII", S. Block, G. J. Piermarini and C. E. Weir, National Bureau of Standards, Washington, D. C.

H-12: "Ice-Like Phases in the NH_4F System", L. D. Calvert, M. A. Nabar and E. Whalley, Division of Applied Chemistry, National Research Council, Ottawa, Ontario

Wednesday Evening, June 30

A.C.A. SESSION K: EXPERIMENTAL AND COMPUTATIONAL AUTOMATION (W. C. Hamilton presiding) :

K-1: "The Oak Ridge Computer-Controlled X-ray Diffractometer", W. R. Busing, R. D. Ellison and H. A. Levy, Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

K-2: "Automatic Diffractometry in a Real Time Multiprogramming Digital Control System", D. R. Fitzwater, D. McFarland and R. M. Stewart, Iowa State University, Ames, Iowa.

K-3: "Experience with the Supper-Pace Automatic Diffractometer", O. Borgen and L. K. Steinrauf, Department of Biochemistry, School of Medicine, Indiana University, Indianapolis, Indiana.

K-4: "An Inexpensive Computer-Controlled Diffractometer System", G. E. Gurr, Minnesota Mining and Manufacturing Company, St. Paul, Minnesota.

K-5: "Procedures for Automated Plotting of Stereoscopic Crystal-Structure Illustrations", C. K. Johnson, Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Thursday Morning, July 1

A.C.A. SESSION M: INORGANIC AND INTERMETALLIC STRUCTURES (A. Zalkin presiding) :

M-1: "Crystal Structure of Europium Silicate, Eu_3SiO_5, A low Temperature Ferromagnetic", J. E. Weidenborner, N. R. Stemple, and Y. Okaya, I.B.M. Watson Research Center, Yorktown Heights, New York.

M-2: "3-Dimensional Study on the Structure of Cesium Pentachlorocobalt, $Cs_3 CoCl_5$", N. R. Stemple and Y. Okaya, I.B.M. Watson Research Center, Yorktown Heights, New York.

M-3: "Hydrogen Bonding and Disorder in $(NH_4)_2Si F_6$ and $(NH_4)_2 SO_4$", E. O. Schlemper and W. C. Hamilton,

Department of Chemistry, Brookhaven National Laboratory, Upton, New York.

M-4: "Additional Refinement of Two Ionic Polysulfide Structures", J. S. Blank and J. Donohue, University of Southern California, Los Angeles, California; and S. C. Abrahams, Bell Telephone Laboratories Incorporated, Murray Hill, New Jersey.

M-5: "The Crystal Structure of ScB_2C_2", G. S. Smith, Q. Johnson and P. C. Nordine, Lawrence Radiation Laboratory, University of California, Livermore, California.

M-6: "The Structure of Yttrium Hectoboride ($\sim YB_{100}$)", S. M. Richards and J. S. Kasper, General Electric Research Laboratory, Schenectady, New York.

M-8: "Neutron Diffraction Study of the Nowotny-Phase $Mo_{<5}Si_3C_{<1}$", E. Parthe and W. Jeitschko, University of Pennsylvania, Philadelphia, Pennsylvania; and V. Sadagopan, Massachusetts Institute of Technology, Cambridge, Massachusetts.

M-9: "The Crystal Structure of Mn_4Si_7", M. H. Mueller and H. W. Knott, Argonne National Laboratory, Argonne, Illinois.

M-10: "Cerium-Magnesium Intermetallic Compounds", Q. Johnson and G. S. Smith, Lawrence Radiation Laboratory, University of California, Livermore, California.

Thursday Afternoon, July 1,

A.C.A. SESSION N: STRUCTURE SOLVING AND REFINEMENT (W. R. Busing presiding):

N-1: "The Role of Conditioning in Phase Determination", H. Hauptman, U. S. Naval Research Laboratory, Washington, D. C.

N-2: "The Determination of Molecular Location", P. Tollin, University of St. Andrews, Queen's College, Dundee, Scotland.

N-3: "The Superposition Frequency Method and Related Techniques", B. T. Gorres and G. G. Gaertner,

Minnesota Mining and Manufacturing Company, St. Paul, Minnesota.

N-4: "Applications of the Superposition Frequency Determination Method", G. G. Gaertner and B. T. Gorres, Minnesota Mining and Manufacturing Company, St. Paul, Minnesota.

N-4S (SPECIAL INVITED PAPER): "Use of Neutron Anomalous Scattering for Phase Determination", S. Ramachisa, Oxford University, Oxford, England.

N-5: "The Separation of Torsional Motion from the Overall Vibration of the Molecular Frame in Electron Diffraction", J. Karle, U. S. Naval Research Laboratory, Washington, D. C.

N-6: "Extension of Intensity Data by Means of the Patterson Function", S. Raman and J. L. Katz, X-ray Laboratory, Department of Physics, Rensselaer Polytechnic Institute, Troy, New York.

N-7: "Treatment of Accidentally Absent Reflections in Least Squares Refinement of Crystal Structures", V. Vand and A. J. Dunning, Pennsylvania State University, University Park, Pennsylvania.

Thursday Evening, July 1

BANQUET: Afterdinner speech by A.C.A. Past President, H. T. Evans, Jr.

Friday Morning, July 2

A.C.A.-M.S.A. JOINT SESSION JB: MINERAL AND INORGANIC STRUCTURES (M. J. Buerger presiding):

JB-2: "Comparison of the Crystal Structures of Binnite, $Cu_{12}As_4S_{13}$, and Tetrahedrite, $Cu_{12}Sb_4S_{13}$", B. J. Wuensch, Ceramics Division, Department of Metallurgy, Massachusetts Institute of Technology, Cambridge, Massachusetts; Y. Takeuchi, Mineralogical Institute, Faculty of Science, University of Tokyo, Tokyo, Japan; and W. Nowacki, Mineralogical-Petrographical Institute, University of Bern, Bern, Switzerland.

JB-3: "A Refinement of the Structure of Lorandite, $TlAsS_2$", C. R. Knowles, Department of Geophysical Sciences, University of Chicago, Chicago, Illinois.

JB-4: "The Crystal Structure of Melanopnlogite, a Low Temperature Cubic Polymorpn of SiO_2", D. E. Appleman, U. S. Geological Survey, Washington, D. C.

JB-5: "A Phenocite-Spinel Inversion in Lithium Aluminum Germanate", A. M. Gaines, A. J. Perotta and D. A. Stepnenson, Department of Geophysical Sciences, University of Chicago, Chicago, Illinois.

JB-7: "The Crystal Structure of Copper (II) Sulfate Trihydrate", R. Zahrobsky and W. H. Baur, University of Pittsburgh, Pittsburgh, Pennsylvania.

JB-8: "The Imperfect Structure of Excess Nitrogen TiN", M. E. Straumanis, C. A. Founce and W. J. James, Materials Research Center, University of Missouri, Rolla, Missouri.

JB-9: "The Systematic Description and Identification of Mica Polytypes", M. Ross, D. R. Wones and H. Takeda, U. S. Geological Survey, Washington, D. C.

PAPERS OF PARTICULAR INTEREST TO THE WRITER

Although each of the papers attended by the writer was of interest to him to some degree, only certain ones were directly related to his work at the Mines Branch. Brief summaries of these papers are included in this section of this report.

A-2: "Peaks and Centroids in Accurate Lattice-Parameter Determination", A. J. C. Wilson, University College, Cardiff, Wales, and Georgia Institute of Technology, Atlanta, Georgia.

Both the peak and the centroid have advantages and disadvantages as measures of diffraction positions. Experimental considerations favour peaks, but corrections are easier to calculate and are more fully

investigated for centroids. Both require intensity measurement over an appreciable range of angle, and each measurement is subject to systematic experimental error and statistical fluctuation.

The peak position is statistically very unstable, and in practice some method of smoothing must be adopted. Objective smoothing requires access to a computer, and smoothing generally introduces some bias because of the asymmetry of the line profile. Smoothed peaks require fewer measurements than centroids, are readily determined for moderately overlapping lines, and are less affected by aberrations at high angles. The disadvantage in using peaks is the lack of complete investigation of the geometrical aberrations, especially in the lower part of the 2θ range.

Centroids have the advantages of objectivity, statistical stability and fully investigated aberrations. Each line requires measurements over a wide angular range, however, and even slight overlapping is troublesome. Although the physical aberrations are large at high angles, these lines are less necessary for lattice-parameter determination.

In the last few years there have been serious attempts at lattice-parameter determination by both approaches. Differences amount to a few parts per hundred thousand, and are probably chiefly attributable to deficiencies in the wavelength data.

A-5: "Intrinsic and Systematic Multiple Diffraction", R. D. Burbank, Bell Telephone Laboratories Incorporated, Murray Hill, N. J.

The conditions under which multiple diffraction can occur have been examined for the single crystal orienter technique and for the precession camera technique. These are compared with the conditions found for normal beam and equi-inclination techniques by Zachariasen, and by Fankuchen et al. For the precession camera, if a crystal is oriented with a symmetry axis parallel to, or a symmetry plane normal to, the spindle axis, multiple diffraction can occur under certain conditions. If the precession angle $\bar{\mu}$ is set at $\bar{\mu} = \cos^{-1}(d^*/2)$, where d^* is the reciprocal lattice spacing from the zero level to an upper level, then all reflections on the zero level are recorded under conditions of triple diffraction. Multiple diffraction can be created or avoided at will by the choice of $\bar{\mu}$, and this should permit direct observation of the effects of multiple diffraction on intensities.

A-8: "Variance of Absorption Effects Observed in Integrated Intensity Measurements of Sodium Chloride and Silicon Single Crystals", G. J. Klems, Republic Steel Corporation, Research Centre, Independence, Ohio; and C. J. Polk, Department of Metallurgical Engineering, Illinois Institute of Technology, Chicago, Illinois.

A standard Hilger-Watts diffractometer was modified by the addition of a crystal monochromator mounted in the path of the incident X-ray beam. The intensities of the incident beam and the beam diffracted by a small single crystal mounted on the diffractometer were continuously and simultaneously monitored by a dual scintillation detector-counter system. Following calibration this enabled the

measurement of "true integrated intensities". Absolute intensities rather than semi-qualitative were calculated, with later conversion to relative intensities on an absolute scale. Among the anomalous absorption effects that were noted, the following appeared to be the most important, and directly applicable to problems encountered at the Mines Branch. It was observed that a 0.005 mm difference in specimen thickness can result in a 3-5% difference in intensity. The desirability of spherical specimens is obvious from this effect.

JA-2: "X-ray Diffraction at Ultra-High Pressure and Temperature", W. G. Field, Air Force Cambridge Research Laboratory, L. G. Hanscom Field, Bedford, Massachusetts.

X-ray diffraction studies were made at pressures up to 100 kilobars and temperatures to 1000°C by a combination of a high power rotating-anode X-ray tube and a tetrahedral anvil press. The data were recorded either by a film camera or counter. As the sample is confined by the gasketing material, experiments can start with the liquid phase. The magnitude of the pressure permits data to be obtained on essentially any material, and the pressure and temperature ranges are such as to permit studies of vital interest to mineralogists and geophysicists. The speaker also stated that the equipment is suitable for the measurement of Mössbauer effect.

JA-3: "The Crystal Substructure in BeO", D. K. Smith and H. W. Newkirk, Lawrence Radiation Laboratory, University of California, Livermore, California.

Single crystals of beryllium oxide were studied by various techniques, and several substructural features were observed which were

related to growth operation. None of these features was observed in the optical microscope. Since this compound has the wurtzite structure, the techniques described might be useful in the zinc sulphide studies of the Mineral Sciences Division.

F-7: "Data for $LaTaO_4$ and $PrTaO_4$, A New Structure Type, and a Series of New Compounds with the $PbNb_2O_6$ Structure, of the Composition $K_{0.5}M_{0.5}Ta_2O_6$, where M is a Rare Earth", G. M. Wolten and A. B. Chase, Aerospace Corporation, Los Angeles, California.

The ortho-niobates of all trivalent rare earths and the ortho-tantalates of the rare earths from Nd through Lu have a structure similar to that of wolframite. These compounds undergo a phase transformation to a scheelite-related structure at elevated temperatures. During the preparation of the ortho-tantalates, several meta-tantalates were obtained, and these are isomorphous with the high-temperature form of lead meta-niobate, which can be considered to be a superlattice of the perovskite structure. The work described may be of interest to those in the Physical Chemistry Section who are working on niobates and tantalates.

F-10: "The Magnetic Structures of Fe_2SiO_4 and Mn_2SiO_4", D. E. Cox and B. C. Frazer, Brookhaven National Laboratory, Upton, New York; I. Almodovar and M. I. Kay, Puerto Rico Nuclear Center, Mayaguez, Puerto Rico.

The magnetic structures present in Fe_2SiO_4 and Mn_2SiO_4 have been determined from a neutron diffraction study of single crystal and polycrystalline specimens. The use of Belov's magnetic space groups is recommended rather than Bertaut's scheme. Although no neutron

diffraction work is done in the writer's laboratory, the discussion arising from this paper was very informative.

H-1: "Crystal Structure of Ferroelectric Lithium Metaniobate, $LiNbO_3$", S. C. Abrahams, J. M. Reddy and J. L. Bernstein, Bell Telephone Laboratories Incorporated, Murray Hill, New Jersey.

A completely new structure analysis was made of this compound since earlier work was considered inexact. Analysis of the three-dimensional Patterson function gave all atomic positions, and a mechanism for the ferroelectricity was proposed in terms of the crystal structure. It was stated that a "single-domain single-crystal" specimen was used for this investigation. The discussion of the paper consisted of a heated argument between S. C. Abrahams and J. D. H. Donnay concerning the use of the terms "single-domain", "single-crystal" and "single-domain single-crystal". The argument was not resolved.

H-2: "Non-Centrosymmetric Structures in the Hexagonal Ferrite Group", J. A. Kohn and D. W. Eckart, U. S. Army Electronics Laboratories, Fort Monmouth, New Jersey.

Single-crystal X-ray studies of the hexagonal ferrites have characterized over 40 mixed-layer structures and polytypes. These phases are hexagonal or rhombohedral and are derived by the c-axis stacking of different structure blocks in varying ratios and permutations. Fundamentally they are all related to both the $BaFe_{12}O_{19}$ and the spinel structures. All the crystals appeared to be perfect, with no indication of random layering. This paper points out the complexities involved in the studies of barium and other ferrites, and is appropriate to the work being done in Mineral Sciences Division.

K-1: "The Oak Ridge Computer-Controlled X-ray Diffractometer", W. R. Busing, R. D. Ellison and H. A. Levy, Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

A computer-controlled Picker X-ray diffractometer operating at high speeds was described. The advantages of the combination of various types of equipment at Oak Ridge should be investigated before a final decision is made on computerizing the existing equipment in the X-ray Laboratory of Mineral Sciences Division.

K-3: "Experience with the Supper-Pace Automatic Diffractometer", O. Borgen and L. K. Steinrauf, Department of Biochemistry, School of Medicine, Indiana University, Indianapolis, Indiana.

The difficulties encountered in the use of the Supper-Pace combination of equipment, and the means of overcoming them were described. Of particular interest to the writer of this report were the problems encountered in crystal alignment, and private discussion with the speaker after the technical session provided the writer with answers to several questions. In the opinion of the speaker the systematic errors present are probably due to severe alignment problems. The speaker was sharply critized at the end of his talk by several who accused him of selling his equipment short. The speaker agreed that neither the diffractometer nor the computer were completely at fault, but also stated that he felt that it was valuable to report his failures as well as successes, in order to benefit others who might encounter similar problems.

N-6: "Extension of Intensity Data by Means of the Patterson Function", S. Raman and J. L. Katz, X-ray Laboratory, Department of Physics,

Rensselaer Polytechnic Institute, Troy, New York.

A method of reorganizing Patterson data was described by the author. Additional information can be obtained by performing these modifications. The resulting discussion included a statement by A. L. Patterson, himself, stating that he approved highly of this method of analysis.

N-7: "Treatment of Accidentally Absent Reflections in Least Squares Refinement of Crystal Structures", V. Vand and A. J. Dunning, Pennsylvania State University, University Park, Pennsylvania.

The methods commonly used for inclusion of accidentally absent reflections in structure determinations is discussed and critized. It was pointed out that the least squares method cannot be used when Gaussian and non-Gaussian distributions are combined. An alternate method was proposed which combined the correct procedure with the most economical computing time. It was stated tnat not only were the previous methods incorrect, but also the standard statistical text books are wrong.

JB-9: "The Systematic Description and Identification of Mica Polytypes", M. Ross, D. R. Wones and H. Takeda, U. S. Geological Survey, Washington, D. C.

The systematic derivation of unit-cell parameters, stacking sequences, space groups and "structural presence criteria" was made for all possible 1-, 2-, 3- and 4-layer mica polytypes. A new method of designating polytypes was proposed, based on vector relationships between adjacent layers. Reference was made to the work of Smith and Yoder, and the new derivation is compatible with their system.

The mica type could not be correlated with the method of crystal growth, and no study was made of ordering within the layers.

GENERAL REMARKS

The joint meeting of the American Crystallographic Association and the Mineralogical Society of America at Gatlinburg was well-organized, in general, and well-attended. Many outstanding papers were presented, although the busy schedule made attendance at all of interest to one person impossible. The opportunities available to talk informally with informed people were as valuable as the technical papers themselves. Continued support of meetings sponsored by either of these two societies is strongly recommended.